A DISCRETE VARIABLE APPROACH FOR INVESTIGATING TUNNELING SPLITTINGS AND VIBRATIONAL WAVE FUNCTIONS IN RARE GAS-ASYMMETRIC TOP HETERODIMERS

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A three dimensional discrete variable representation (DVR) is developed for the general case of a rare gas atom interacting with an asymmetric top molecule and applied to the case of argon-haloethylene heterodimers. The position of the rare gas is specified relative to the principal inertial axis system (in a I^r representation) by the spherical polar coordinates (r, θ, ϕ). While the DVR for r is straightforward, those for θ and ϕ presented particular challenges, which are discussed. In common with all DVR approaches, the present DVR is well suited for systems where the intermolecular potential is calculated on a grid of discrete points and provides easy access to the wave functions in the DVR coordinates. The method is applied to the well-characterized argon-*cis*-1,2-difluoroethylene system and used to predict the tunneling splitting and argon-molecule vibrational wave functions in argon-vinyl chloride for which the molecular structure and rotational spectrum remain a puzzle.